A new method to use Water Pinch Analysis for complex wastewater scenarios

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Water Pinch Analysis
Wastewater/fresh Water Minimization
Complex Wastewater

ABSTRACT
A new method was developed to easily determine process critical concentrations allowing the use of Water Pinch Analysis to minimize the fresh water (FW) requirement of processes dealing with complex wastewater. This method consists in experimentally recycling water within the studied process until some process units get their key performance indicators negatively impacted. This paper provides all the mathematical tools to calculate the critical concentrations of a generic compound called "contaminant X" based on the critical number of recyclings and effectively use Water Pinch Analysis. This developed method was applied to a continuous and mix batch/continuous process with or without storage tanks, and two scenarios where some processes could remove a fraction of "contaminant X", from a biological process for example (such as anaerobic digestion). The Near Neighbour Algorithm had to be slightly modified to be used in pure batch or mix batch/contiguous processes with without storage tank. In all cases, the FW requirement was minimized while guaranteeing that all processes were working at optimal performances.

Introduction
Water Pinch Analysis has been designed by Professor Robin Smith from Manchester University in the mid 1990’s to minimize fresh water (FW) requirement in processes (Foo, 2009). It has been successfully applied in many industries and significantly reduced operating costs, wastewater treatment costs and environmental impacts (Khezri et al., 2010; Mughees and Al-Ahmad, 2015; Mi et al., 2011).

This technique is based on the determination of the maximum re-usage of water (and therefore minimum wastewater discharge) within a process to reduce the need for FW while ensuring that all processes are operating at optimum conditions. This very effective approach requires the determination of the process input and output critical concentrations. Those critical concentrations correspond to the maximum inlet and outlet contaminant concentrations, each process units can tolerate. They have to be maximized in order to minimize the FW requirement (Process Integration Limited, 2012).

Although, several methods have been developed to deal with multiple contaminant scenarios (Wang et al., 2003; Majozi and Gouws, 2009; Mohammadnejad et al., 2012). Water Pinch Analysis is generally more effective at optimizing water re-use in single contaminant water systems (Meng et al., 2014). Moreover, in certain processes, determining the critical contaminants and their concentrations can be very difficult due to the complexity of the involved wastewater. For example, a process that would involve leachate being in contact with water, will have many potential toxic compounds for biological processes (Paxéus, 2000).

To date, there is currently no method to apply Water Pinch Analysis in such cases, i.e. with processes dealing with complex multi-compound containing wash water. This paper introduces a new simple method to overcome this difficulty while allowing the use of Water Pinch Analysis.

Several methods have been developed to determine the minimum FW required such as the water cascade analysis (Foo, 2007), graphical targeting method (Hallale, 2002), or the automated targeting technique for continuous (Ng et al., 2009) and batch processes (Foo, 2010). For batch processes, storage tanks (STk) can be used to store
water from a given interval \( t \), to be used in another interval \( t+k \) with \( k \geq 1 \) (Foo, 2010).

The latest method was chosen due to the ease of programming the algorithms using Microsoft Excel Visual Basic for Application (VBA) and its flexibility. For similar reasons, the Near Neighbour Algorithm (NNA) technique as developed by Prakash and Shenoy (2005) was used to design water networks. NNA has not been adapted yet for batch process with or without Stk, however, this matter was addressed in this paper.

**Research Methods**

For the description of the methodology, the series of processes shown in Figure 1 was considered. Each process \( i \) has a \( F_{i,\text{lin}} \) water demand, and releases \( F_{i,\text{out}} \) defined as a source (with \( F \), a flow in whatever unit as long as consistent). The current flows displayed in the diagram follow the succession of process units. All equations in this article are the authors’ own work.

The concept of the proposed methodology is to perform at lab/pilot or even full-scale, an experiment (designed as main experiment, ME) with recirculation of wastewater and minimum FW addition until one or several processes get their key performance indicators (KPIs) negatively impacted (e.g., conversion, etc.) This has to be carried out in a batch or semi-continuous mode.

On certain cases, however, FW must be added or water being discharged (DW) (equation (1) and (2)) respectively, to maintain a constant volume of water and satisfy process water demands.

\[
\text{if } F_{i,\text{lin}} > \sum_j F_{j,\text{out}} \text{ then } F_{i,\text{lin}} = F_{i,\text{lin}} - \sum_j F_{j,\text{out}} \quad \quad (1)
\]

\[
\text{if } F_{i,\text{out}} > \sum_k F_{k,\text{lin}} \text{ then } F_{i,\text{out}} = F_{i,\text{out}} - \sum_k F_{k,\text{lin}} \quad \quad (2)
\]

Where \( j \) represents the sources fulfilling process demand \( i \), and \( k \) represents the water demands requiring process source \( i \). The horizontal bars indicate the available flow. For example, the available water flow from process 1 going to process 2 is (see Figure 1):

\[
F_{1 \rightarrow 2,\text{out}} = \%P_i \times (F_{i,\text{out}} - D_{i,\text{lin}}) \quad \quad (3)
\]

Another concept introduced here, is the notion of “contaminant \( X \)” which represents a generic contaminant that could affect any of the process. It is important to keep in mind that it cannot be qualified nor quantified. It is assumed that 1 unit of “contaminant \( X \)” is transferred each recycling (\( \Rightarrow 1 \)). To be able to determine the proportion of “contaminant \( X \)” being transferred to the water during each process, the concentration of a measurable indicator compound, \( \text{[ind.]} \) must be monitored at least for the first recycling. This compound should be chosen so that it is not removed or retained by any of the processes. The transfer of \( \text{[ind.]} \) during each process is defined in equation (4).

\[
\text{[ind.]}_i = \text{[ind.]}_i - \sum_j F_{j,\text{out}} \times \text{[ind.]}_j - \sum_k F_{k,\text{lin}} \times \text{[ind.]}_k \quad \quad (4)
\]

Where \( V_{i,f} \) is the final volume of water remaining in process \( i \) (if applicable). The “contaminant \( X \)” transfer ability (in %) of each process \( i \) is defined in equation (5).

\[
\%X_{i,\text{lin}} = \frac{\%\text{[ind.]}_i \times 100}{\sum \%\text{[ind.]}_i} \quad \quad (5)
\]

From these equations, it is possible to calculate the inlet and outlet concentrations of “contaminant \( X \)” (\( [X]_{i,\text{in},n} \) or \( [X]_{i,\text{out},n} \)) at every recycling \( n \) as defined in equation (6) and (7).

\[
[X]_{i,\text{lin},n} = \frac{\sum_j F_{j,\text{out}} \times [X]_{j,\text{out},n} + V_{i,f} \times [X]_{i,\text{lin},n-1}}{\sum_j F_{j,\text{out}} + V_{i,f}} \quad \quad (6)
\]

\[
[X]_{i,\text{out},n} = \frac{\sum_j F_{j,\text{lin}} + V_{i,f} \times [X]_{i,\text{out},n-1} \times \%X_{\text{removal},i}}{\sum_j F_{j,\text{lin}} + V_{i,f}} \quad \quad (7)
\]

Where \( \%X_{\text{removal},i} \) is the percentage of “contaminant \( X \)” removal by process \( i \). Note that \([X]_{i,\text{out},0}=0\) (general), and \([X]_{i,\text{lin},0}=0\) (for the described process).

Once the experiment over and the number of recyclings leading to one or several process failure is determined for each process \( i \): \( n_{\text{critical},i} \), the critical concentrations can be calculated. Because the concentration leading to failure cannot be clearly determined (is it \( [X]_{i,\text{lin},n_{\text{critical},i}} \) or \( [X]_{i,\text{out},n_{\text{critical},i}} \)?), the number of recyclings is taken to \( n \). This could lead to a slightly over-estimation of the FW requirement, but it will ensure process stability.

From this, the Ng and Foo et al. automated targeting Water Pinch Analysis technique described in (Ng et al., 2009) can be used to determine the minimum FW requirement and the pinch point, and the NNA used for network design (Prakash and Shenoy, 2005).

In the situation, a process \( i \) is able to remove a fraction of “contaminant \( X \)” (PR), i.e., with \( \%X_{\text{removal},i} \neq 0 \), such as a biological process (an anaerobic digester for example), it is important to run a parallel experiment (PE) to determine the “contaminant \( X \)” removal. In fact, \( \%X_{\text{removal}} \) drives the minimum FW requirement as shown later in case study 2 (Figure 4). In PE, the recycling experiment is carried out as previously described, except that PR is by-passed.
Note that if PR is critical for the process, water can be diluted (df). If it is assumed that process 3 (see Figure 1) is a PR, equation (6) for process 1 will be re-written:

\[ [X]_{\text{in,1}} = \frac{F_{2-out} + \sum_{i=1}^{n-1} F_{\text{in,1}} \cdot [X]_{\text{out,1}+T} + V_{1,t} [X]_{\text{out,1}}}{F_{2-out} + F_{\text{in}} + V_{1,t}} \]  

(8)

ME and PE are carried out until one or several processes get their KPIs negatively impacted. A solver is then used to determine the \( \%X_{\text{removal,i}} \) of PR, with the objective of minimizing equation (9).

\[ \sum_i (\left( [X]_{\text{in,sum,1}} - [X]_{\text{in,sum,1}} \right)^2) \]  

(9)

Where \( n_{\text{critical,ME}} \) and \( n_{\text{critical,PE}} \) are the number of recyclings leading to one or several process for each process j determined in the main and parallel experiment respectively.

The results from this method can also be applied to minimize the FW requirement of batch or mix batch/continuous processes. The automated targeting Water Pinch Analysis for batch process can be used with or without storage tanks (STk) (foo, 2010). The NNA technique is also suitable for batch processes and is applied for each time intervals \( t-t+1 \).

If the process allows the use of storage tanks i.e. the transfer of water across time intervals, the initial NNA logic needs to slightly be changed. The important NNA rules or statement are (Prakash and Shenoy, 2005):

1. “To satisfy a particular water demand, the source streams to be chosen are the nearest available neighbors to the demand in terms of contaminant concentration.”
2. “all demands below the pinch must have their inlet concentrations equal to the maximum allowable values, whereas demands above the pinch can have inlet concentrations less than their maximum allowable values.”

If 1. does not need to be called into question, it is important that the STk demands receive water at their maximum allowable inlet concentration values regardless their position in relation to the pinch point, as other time intervals require this level of water purity. Therefore, to apply the NNA technique in batch or mix batch/continuous processes with water STk, the following procedure was used:

- All STk demands must be satisfied in priority at their maximum allowable inlet concentration values following the principle of NNA.
- Then “all demands [other than STk demands] below the pinch must have their inlet concentrations equal to the maximum allowable values, whereas demands [other than STk demands] above the pinch can have inlet concentrations less than their maximum allowable values.”

Case study 2 and 3 will be used to illustrate this new constraint on the NNA technique for batch processes with storage tanks.

Results and Discussion

Several hypothetical case studies were used in this work with invented data.

Case study 1: illustration of the new developed method without “contaminant X” removal

Flow data (from Error! Reference source not found. Figure 1) are shown in Table 1. 40 recyclings were carried out in this experiment and 8 L of FW was added each time (from calculation). \( \%X_{\text{removal}} \) is taken equal to 0. The concentration of an inert indicator compound was measured in process outlets. Results are shown in Table 2 with the calculated “contaminant X” transfer abilities.

In this case study, it was found that processes 1, 3, 4, 5 showed signs of failure after 6, 10, 14, 8 recyclings respectively while process 2 was still not affected when the experiment was stopped. As a reminder, critical concentrations were calculated from n-1. The calculated critical concentrations are given in Table 3 and were obtained from Figure 2.

Using Water Pinch Analysis, it was found that 2.73 L of FW needed to be added per recycling, and therefore the same volume to be disposed. This corresponds to a reduction of 66% from the water added during the recycling experiment which is due to an optimum re-allocation of the FW addition. The design of the final water network is presented in Figure 3 with the different water re-allocations.
Figure 1. Initial process flow diagram for case study 1

Table 1. Limiting data for case study 1

<table>
<thead>
<tr>
<th>Process</th>
<th>Volume of water in process**</th>
<th>Demand</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>D1</td>
<td>S1</td>
</tr>
<tr>
<td>2</td>
<td>3</td>
<td>D2</td>
<td>S2</td>
</tr>
<tr>
<td>3</td>
<td>0</td>
<td>D3</td>
<td>S3</td>
</tr>
<tr>
<td>4</td>
<td>2</td>
<td>D4</td>
<td>S4</td>
</tr>
<tr>
<td>5</td>
<td>4</td>
<td>D5</td>
<td>S5</td>
</tr>
</tbody>
</table>

*in L^3 per recycle, **in L. %P1=25%

Table 2. "Contaminant X" transfer ability calculation for case study 1 (\%X_{\text{removal}}=0)

<table>
<thead>
<tr>
<th>Process</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>[Ind] (in g/L)</td>
<td>15.0</td>
<td>22.5</td>
<td>11.3</td>
<td>11.3</td>
<td>7.5</td>
</tr>
<tr>
<td>(\Rightarrow) (in g)</td>
<td>45.0</td>
<td>123.8</td>
<td>0</td>
<td>33.8</td>
<td>22.5</td>
</tr>
<tr>
<td>(\Rightarrow) (in %)</td>
<td>20</td>
<td>55</td>
<td>0</td>
<td>15</td>
<td>10</td>
</tr>
</tbody>
</table>

Table 3. Critical concentrations for case study 1 determined by the developed method (\%X_{\text{removal}}=0)

<table>
<thead>
<tr>
<th>Demand</th>
<th>([X]_{\text{in}}) (unit/L)</th>
<th>Source</th>
<th>([X]_{\text{out}}) (unit/L)</th>
</tr>
</thead>
<tbody>
<tr>
<td>D1</td>
<td>0.102</td>
<td>S1</td>
<td>0.169</td>
</tr>
<tr>
<td>D2</td>
<td>0.140</td>
<td>S2</td>
<td>0.231</td>
</tr>
<tr>
<td>D3</td>
<td>0.114</td>
<td>S3</td>
<td>0.114</td>
</tr>
<tr>
<td>D4</td>
<td>0.120</td>
<td>S4</td>
<td>0.145</td>
</tr>
<tr>
<td>D5</td>
<td>0.115</td>
<td>S5</td>
<td>0.126</td>
</tr>
</tbody>
</table>
Figure 2. Inlet and outlet concentrations for Case study 1. + corresponds to process inlet concentration, - corresponds to process outlet concentration. Dash lines correspond to the maximum inlet critical concentrations (%Xremoval=0)

Figure 3. Optimized water network for case study 1 (all numbers are in L) (%Xremoval=0)

Case study 2: Illustration of the new developed method with “contaminant X” removal

Data from case study 1 was used again with the same n_critical, but it will now be assumed that process 3 is able to remove a fraction of “contaminant X” to be determined. To calculate the minimum FW requirement, it is important to evaluate %X_{removal} as seen in Figure 4. In fact, this really drives the amount of FW requirement. Higher %X_{removal} means that cleaner water is released from process 3 which can thus be re-used to fill demands with low critical “contaminant X” concentration.

PE was carried out by by-passing process 3 and 60 recyclings were conducted. Df was taken equal to 5 to ensure process stability. For PE it was found that processes 1, 4, 5 showed signs of failure after 6, 39 and 8 recyclings respectively while process 2 was still not affected when the experiment was stopped. Calculated critical concentrations for PE are given in Table 4.

A solver was then used to determine %X_{removal,3} for the ME to minimize equation (9). %X_{removal,3} was found be equal to 60% and 1.09 L of FW needed to be added. Optimum water network is shown in Figure 85 and correspond to a FW demand reduction of 86%.
Figure 4. Impact of percentage “contaminant X” removal by process 3 on overall fresh water requirement at fixed $n_{\text{critical}}$

Table 4. Critical concentrations for PE determined by the developed method (for case study 2)

<table>
<thead>
<tr>
<th>Demand</th>
<th>$[X]_{\text{in}}$ (unit/L)</th>
<th>Source</th>
<th>$[X]_{\text{out}}$ (unit/L)</th>
</tr>
</thead>
<tbody>
<tr>
<td>D1</td>
<td>0.063</td>
<td>S1</td>
<td>0.130</td>
</tr>
<tr>
<td>D2</td>
<td>0.127</td>
<td>S2</td>
<td>0.219</td>
</tr>
<tr>
<td>D4</td>
<td>0.093</td>
<td>S4</td>
<td>0.118</td>
</tr>
<tr>
<td>D5</td>
<td>0.097</td>
<td>S5</td>
<td>0.108</td>
</tr>
</tbody>
</table>

Figure 5. Optimized water network for case study 2 (all numbers are in L) ($\%X_{\text{removal}}=60\%$)
Case study 3: Illustration of the new developed method with a semi-real situation

The data for the case study 3 are derived and modified from Vaurs (2018). It consists of washing 2 tonnes/day of the organic fraction of municipal solid waste (OFMSW) coming at 50% moisture with 6 tonnes of hot water. This solubilizes the food waste fraction and releases a wastewater rich in chemical oxygen demand (COD) for biogas production in an anaerobic digestion (AD) reactor. The insoluble organic fraction (40% of the initial dry weight) is processed in a biological process (undefined here for confidential reasons) at 70% moisture (no water addition).

A unit of “contaminant X” is transferred during the washing. The AD reactor is assumed to be able to remove some “contaminant X” but not the biological process (BP). 3 KPIs will be looked at in this case study: the COD removal and methane yield from the AD reactor and the conversion yield from the BP. The methodology described earlier was applied on this case study. The “clean” water by AD was re-used for the washing process but 0.4 tonnes of water still needed to be added for every washing (no water leaves BP).

Results are shown in Figure 6. COD removal and methane yield decreased with the number of recycling, probably due to the accumulation of “contaminant X” in the wastewater. 15 recyclings appeared to be a good compromise between process performance and the level of dirtiness of the water. Regarding BP (Figure 6B), the conversion yield remained relatively constant (averaging 85%) but after the 16.5th recycling the conversion sharply decreased. If the critical recycling number i.e. 16.5 is not an integer is because occasionally FW was added in the BP to maintain the water at target volume.

A PE was run to determine the “contaminant X” removal by AD where the AD was skipped. To mimic the COD removal by AD, the outlet from the washing was diluted to match the COD removal given by A. During PE, BP performances were seriously affected after 47 recycling, which corresponded to a \([X]_{1,\text{in}}=0.1747\) unit tonne\(^{-1}\). Note that the washing process will never be affected by “contaminant X”, so \([X]_{1,\text{in}}\) and \([X]_{1,\text{out}}\) could in principle be very high. The water contained in the washed OFMSW (Figure 6A.), however, must not be higher than \([X]_{3,\text{in}}\), so \([X]_{1,\text{out}}\) is forced to \([X]_{3,\text{in}}\) and \([X]_{1,\text{in}}\) is calculated from it using equation 7.

Figure 6. A) Methane yield and COD removal by anaerobic digestion and B) conversion yield by the biological process for case study 3
Table 5. Limiting data for case study 3

<table>
<thead>
<tr>
<th>Number</th>
<th>Process</th>
<th>Volume of water in process**</th>
<th>Demand</th>
<th>Source</th>
<th>Flow*</th>
<th>Name</th>
<th>Flow*</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Washing process</td>
<td>0a</td>
<td>D1</td>
<td>S1</td>
<td>7</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>Anaerobic digestion</td>
<td>0b</td>
<td>D2</td>
<td>S2</td>
<td>5.6</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>Biological process</td>
<td>0</td>
<td>D3</td>
<td>S3</td>
<td>0</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*a* in tonne day⁻¹  **b** in tonne, a=all water is drained after the washing, b=considered negligible. In the recycling experiment, 5.6 tonnes day⁻¹ from S1 was going to D2 and 1.4 was going to D3.

Figure 7. Optimized water network for case study 3. All in tonne /day. * for solid flows, ** for wastewater flows (%X<sub>removal</sub>=77%)

Table 6. Limiting data for case study 4

<table>
<thead>
<tr>
<th>Process</th>
<th>Volume of water in process**</th>
<th>Demand</th>
<th>Period</th>
<th>Source</th>
<th>Flow*</th>
<th>T&lt;sub&gt;start&lt;/sub&gt;</th>
<th>T&lt;sub&gt;end&lt;/sub&gt;</th>
<th>Period</th>
<th>Source</th>
<th>Flow*</th>
<th>T&lt;sub&gt;start&lt;/sub&gt;</th>
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<tr>
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<td>1</td>
<td>D1</td>
<td>5</td>
<td>Cont.</td>
<td>S1</td>
<td>5</td>
<td>Cont.</td>
<td></td>
<td></td>
<td></td>
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</tr>
<tr>
<td>2</td>
<td>3</td>
<td>D2</td>
<td>20</td>
<td>1</td>
<td>3</td>
<td>S2</td>
<td>15</td>
<td>1</td>
<td>3</td>
<td></td>
<td></td>
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<tr>
<td>3</td>
<td>7</td>
<td>D3</td>
<td>7</td>
<td>3</td>
<td>3</td>
<td>S3</td>
<td>7</td>
<td>3</td>
<td>6</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*a* in L/ per recycle, ** in L. T<sub>start</sub> and T<sub>end</sub> in hours, cont.=continuous

Case study 4: Application of the new developed method for mix continuous/batch processes

Limiting data for case study 4 are shown in Table 6. In this case study, no “contaminant X” was removed by any of the processes. 15 L of FW was added every recycling (only 5 L from process 1 could be transferred to process 2).

The concentration of an inert indicator compound was measured in process outlets. Results are shown in Table 7 with the calculated “contaminant X” transfer abilities. Process 1, 2 and 3 presented signs of failure after 10, 20 and 6 recyclings which correspond to the critical concentrations given in Table 7. Water minimization was carried out with and without water STk using Foo’s automated targeting Water Pinch Analysis for batch processes (Foo, 2010), and 15.65 and 15.48 L of FW needed to be added per recycling respectively. 10.65 and 10.48 L of wastewater needed to be disposed. Only 1 STk was needed with a working volume of 0.35 L. Note that in real scenarios, techno-economic assessments should be carried out determine if the FW reduction with STks justify the extra capital and operating costs (tanks, pumps, energy for pumping, piping etc.).

The designs of the final water networks with or without STks are presented in Figure 8 and Figure 9 with the different water re-allocations.
Table 7. "Contaminant X" transfer ability calculation and critical concentration for case study 4

<table>
<thead>
<tr>
<th>Process</th>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>[Ind] (in g/L) ⇒ (in g)</td>
<td>45</td>
<td>46.3</td>
<td>56.9</td>
</tr>
<tr>
<td>[X] (in %) ⇒ (in g)</td>
<td>270</td>
<td>607.5</td>
<td>472.5</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Demand</th>
<th>Source</th>
<th>Demand</th>
<th>Source</th>
<th>Demand</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>[X] (unit/L)</td>
<td>0.047</td>
<td>0.080</td>
<td>0.025</td>
<td>0.057</td>
<td>0.074</td>
</tr>
</tbody>
</table>

Figure 8. Optimized water network for case study 4 without STk (all numbers are in L), (%X<sub>removal</sub>=0%)

Figure 9. Optimized water network for case study 4 with STks (all numbers are in L), (%X<sub>removal</sub>=0%)
Conclusions
A new method was developed to overtake the challenge of determining the critical concentrations of processes dealing with complex wastewater. This method consists in experimentally recycling water in a process until some units got their KPIs negatively impacted. This method was applied to 4 hypothetical case studies including continuous and mix batch/continuous scenario with or without storage tank and scenario with a process able to remove a fraction of “contaminant X”. Using Water Pinch Analysis, FW addition was minimized while maintaining processes at optimum operating conditions.

Conflict of interest
The authors declare that there is no conflict of interest in this publication.

References


